Exponential Capacity in an Autoencoder Neural Network with a Hidden Layer

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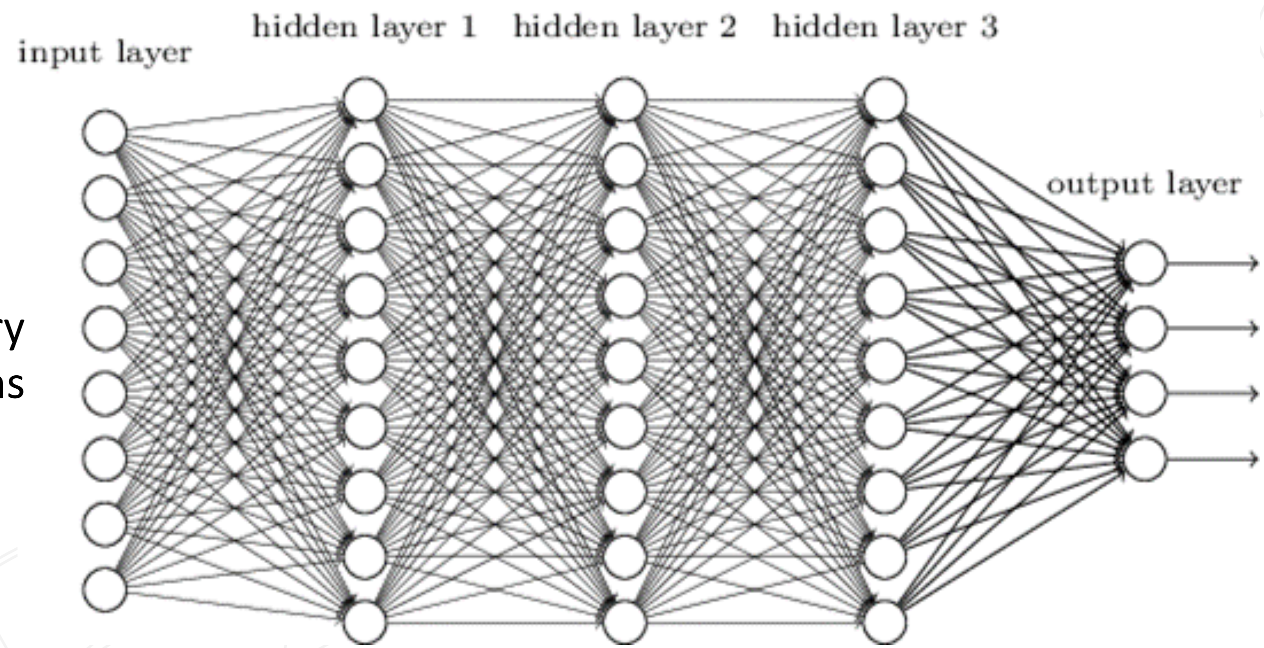
PHYSICS INFORMED MACHINE LEARNING

Santa Fe, NM, Jan 2018

Limits of computations in deep nets?

random binary
input patterns



random binary
output labels

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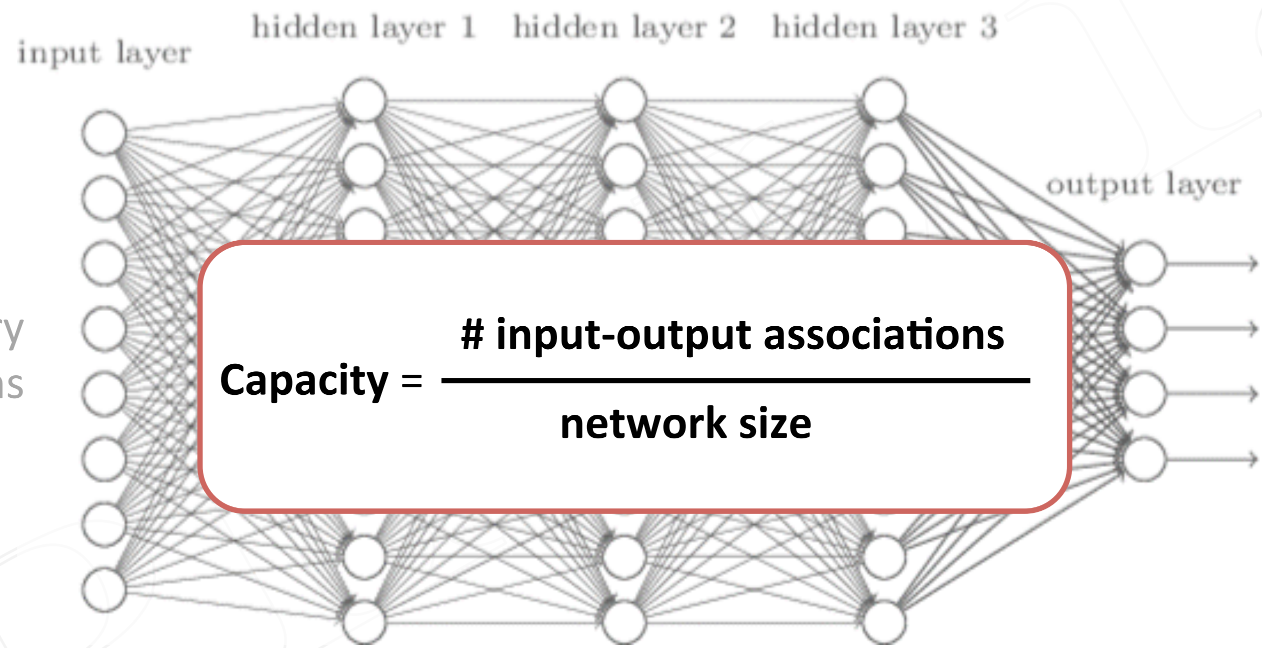
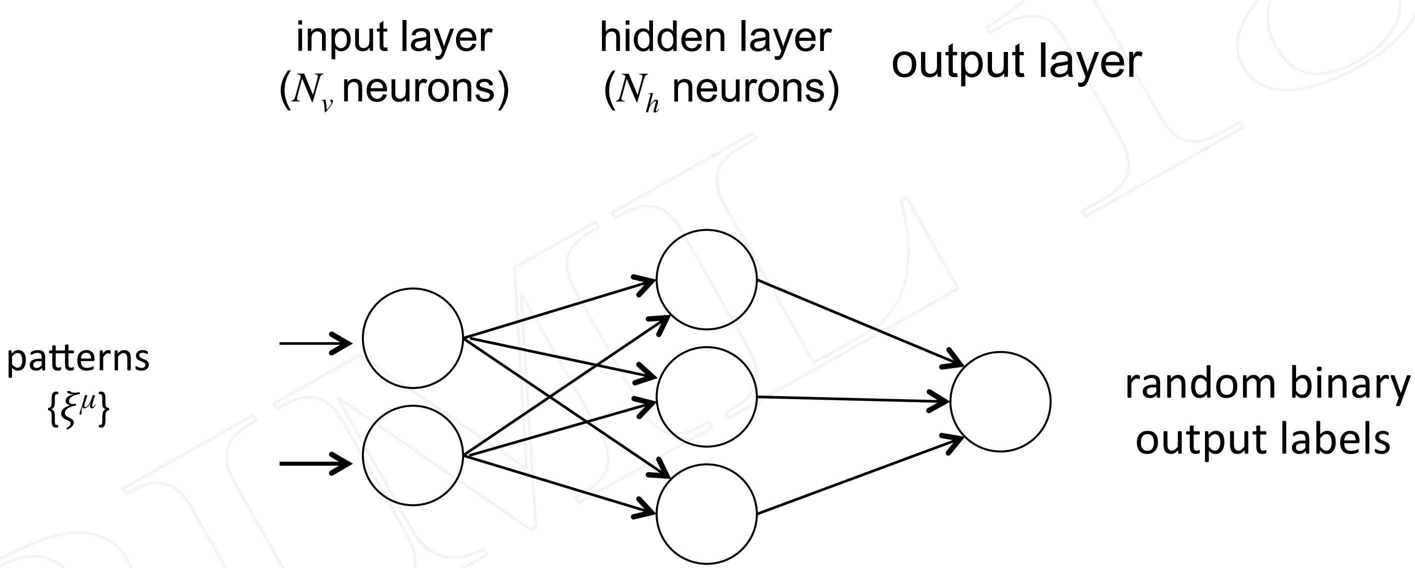


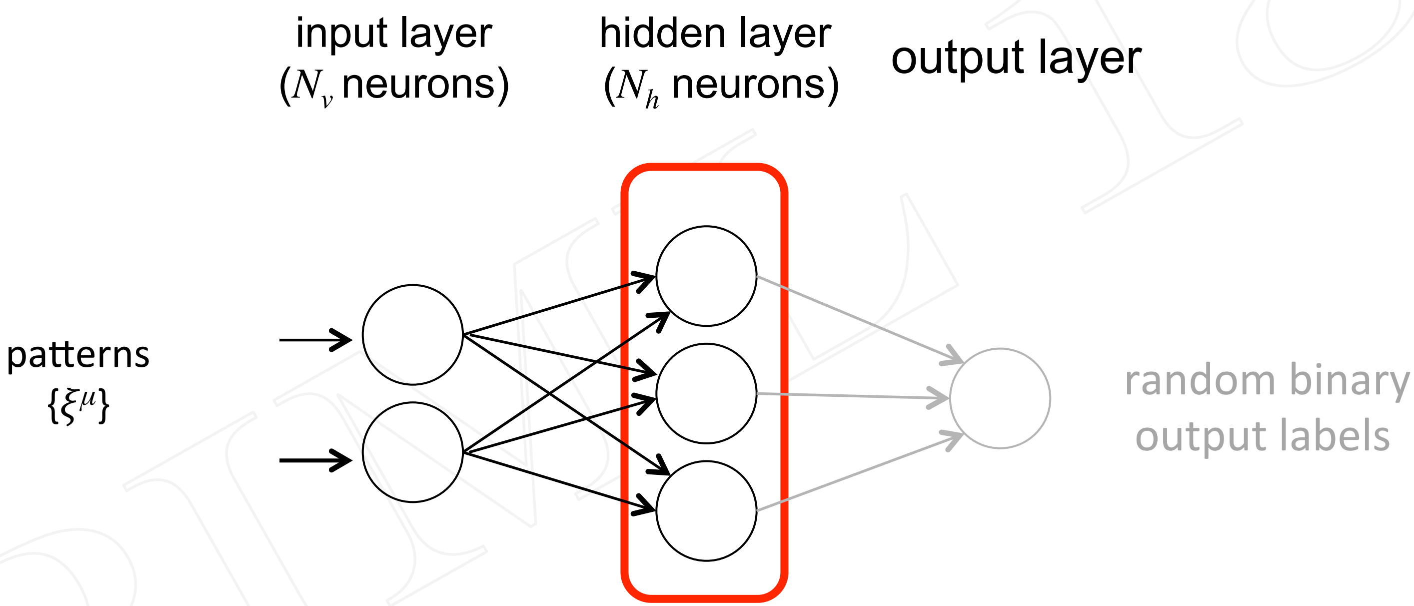
random binary
output labels

$$\text{Capacity} = \frac{\text{\# input-output associations}}{\text{network size}}$$

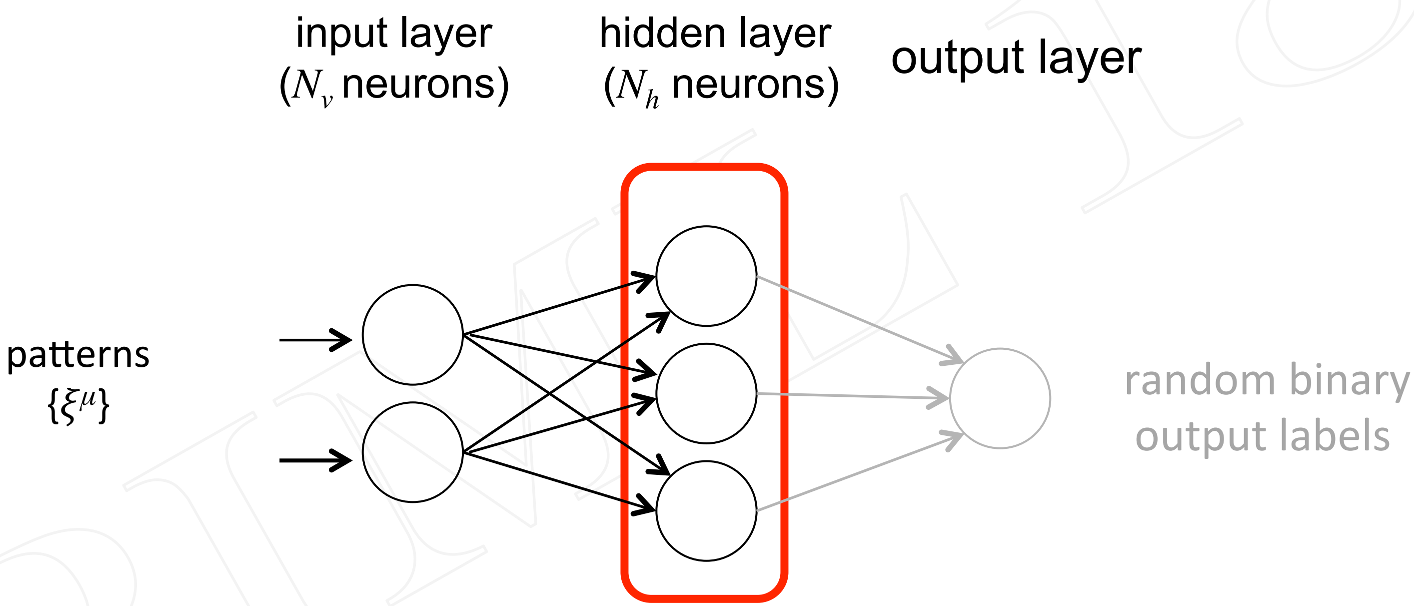
Capacity of multi-layer perceptron (MLP) with one hidden layer?



Investigating internal representation



Expansive (or *overcomplete*) representation

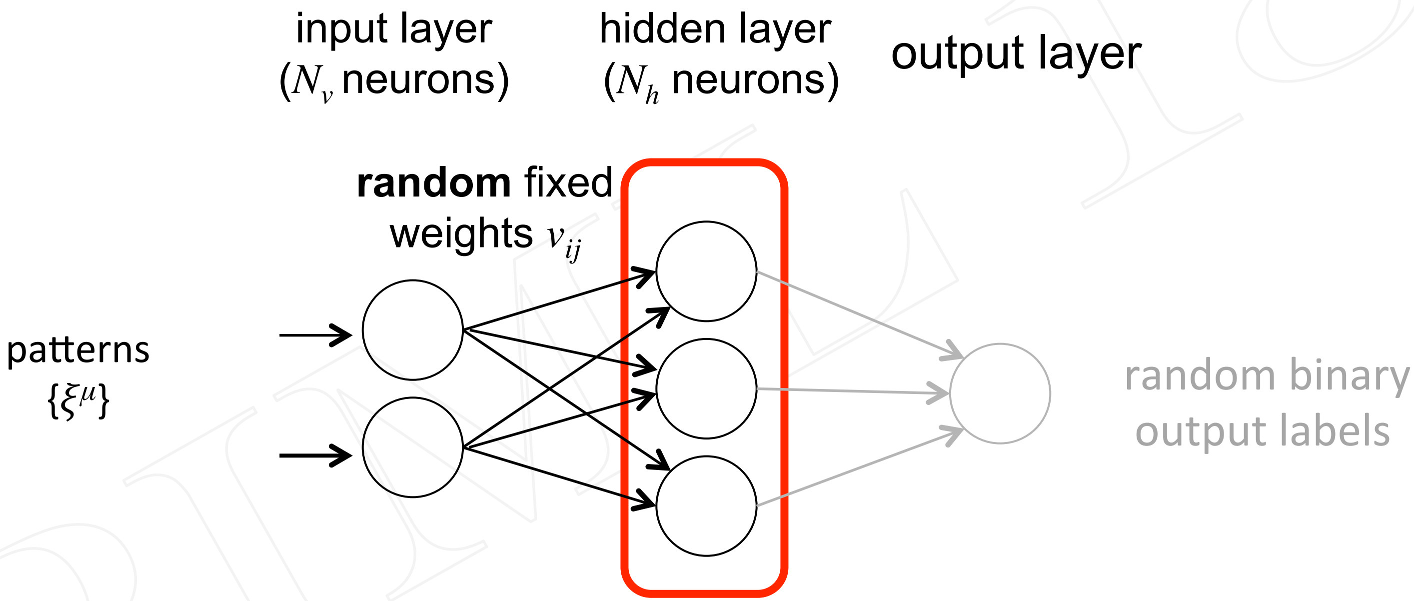


$$\Lambda = \frac{N_h}{N_v} > 1$$

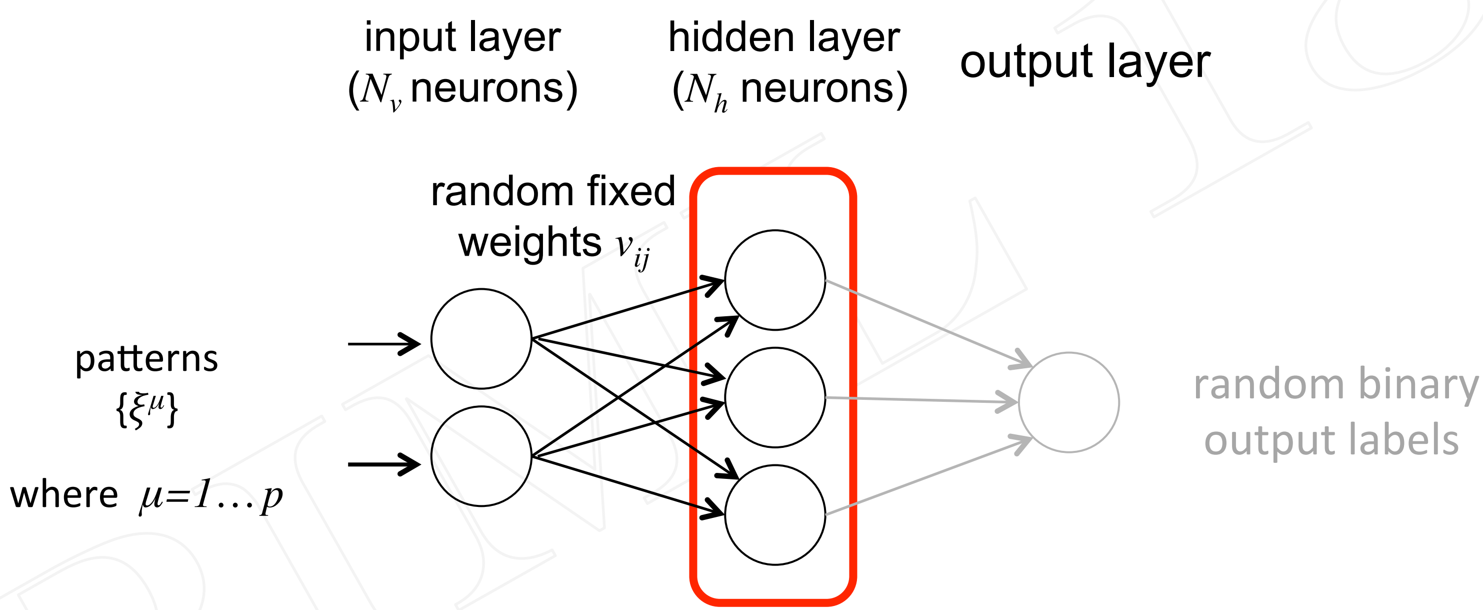
Expansive (or *overcomplete*) representation

Nervous system	Expansion ratio (Λ)
Entorhinal cortex → Dentate gyrus	~ 10
LGN → V1	~ 25
in fly olfactory system: antennal lobe → mushroom body	~ 40
in the cerebellum, mossy fibers → granule cells	$100 \sim 200$
rodent's olfactory bulb → piriform cortex	$\sim 10^3$

Expansive representation with **random** weights

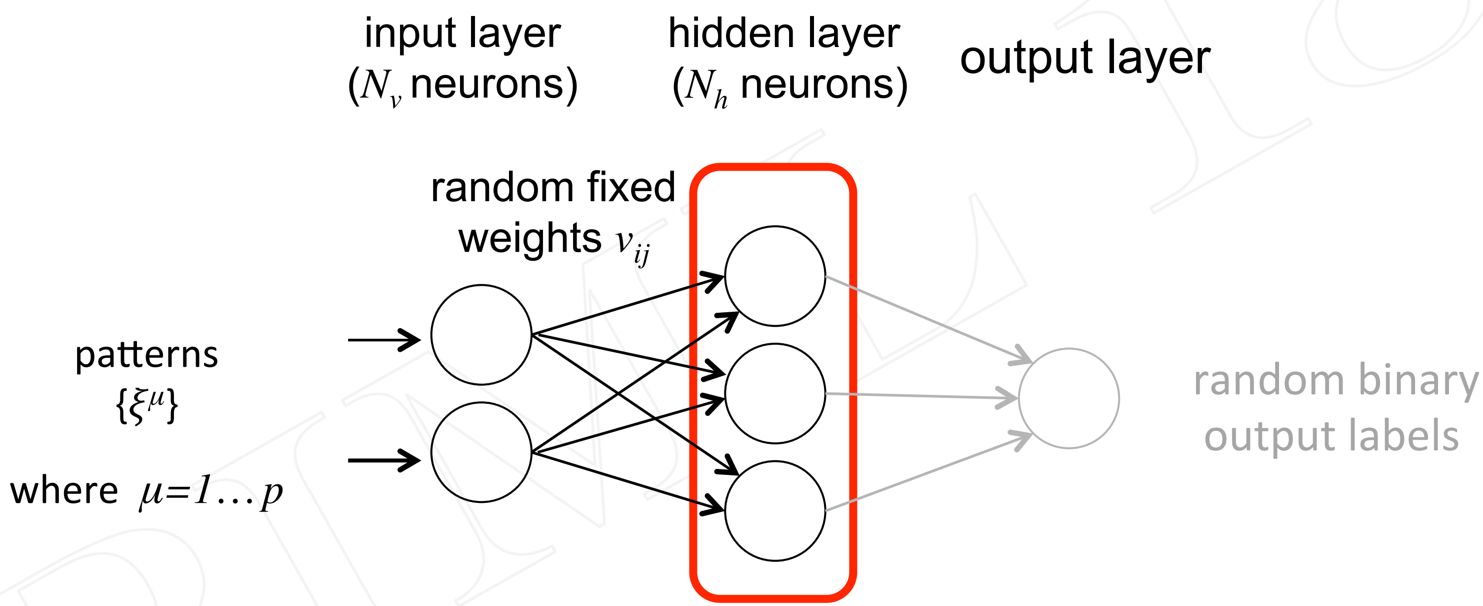


Expansive representation with random weights



How good is random-weight expansive representations?

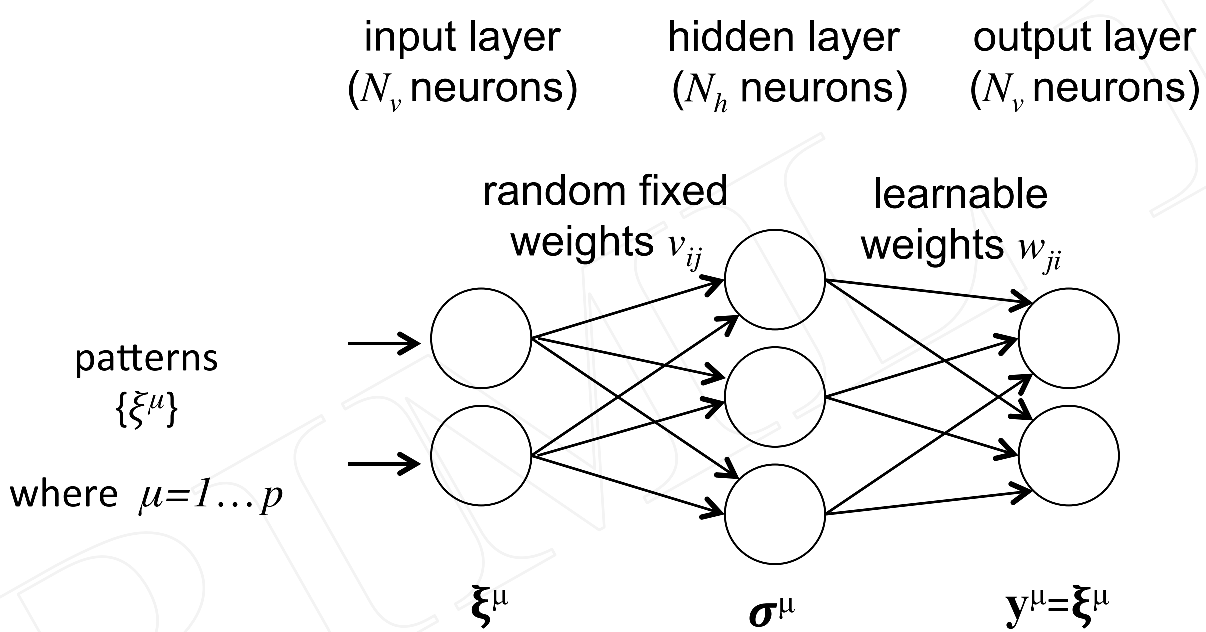
Expansive representation with random weights



How good is ra
expansive repr

How many of input patterns can be reconstructed from this representation?

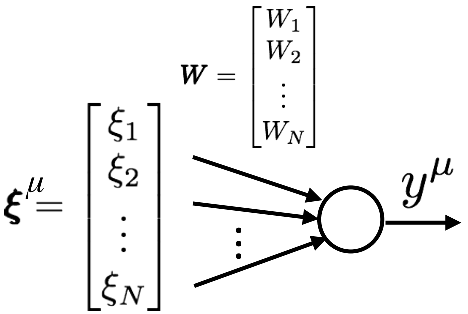
Expansive **autoencoder** with random weights



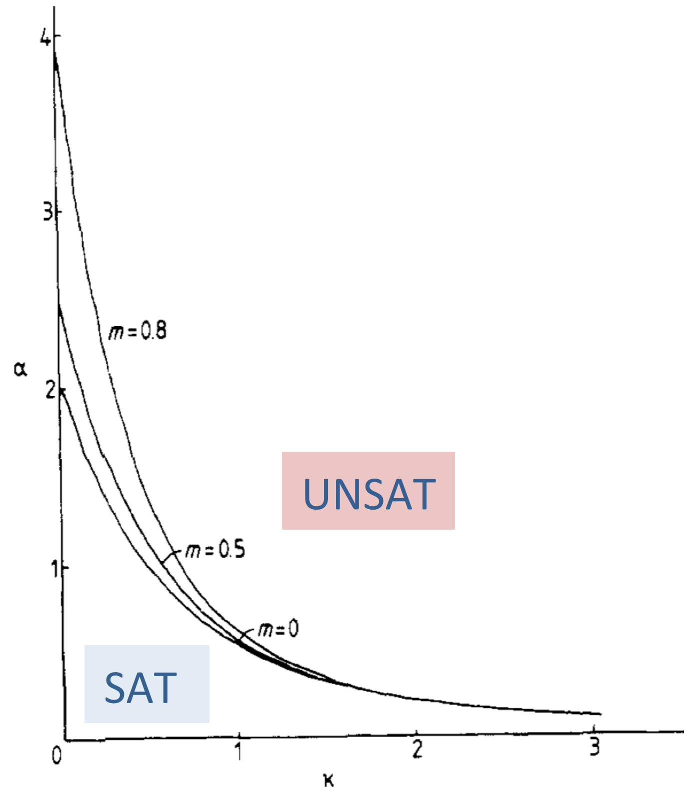
Focus of this talk:

Optimal capacity of expansive autoencoder?

Critical capacity of the perceptron: Gardner approach



$$y^{\mu} = \mathrm{sgn}\left(\frac{\mathbf{w}\cdot\boldsymbol{\xi}^{\mu}}{\sqrt{N}} - \theta\right)$$



Gardner E. (1988) J. Phys. A: Math. Gen.

- Find $\mathbf{w}$ to store a set of random ensemble of input-output pairs $\{ (\boldsymbol{\xi}^{\mu}, d^{\mu}) \}$, $\mu=1\ldots p$ with a robustness κ
- Storage criteria: $\forall \mu, i: \; d^{\mu}\left(\frac{1}{\sqrt{N}}\sum_{i=1}^{N} w_i \xi_i^{\mu} - \theta\right) > \kappa$

Gardner volume ($N \longrightarrow \infty$):

$$\Omega = \int_{\|\mathbf{w}\|^2=N} d^N\mathbf{w} \prod_{\mu=1}^{p} \Theta\left(d^{\mu}\left(\frac{1}{\sqrt{N}}\sum_{i=1}^{N} w_i \xi_i^{\mu} - \theta\right) - \kappa\right)$$

$\langle\!\langle \log(\Omega) \rangle\!\rangle$ averaging over the (quenched) distribution of the patterns

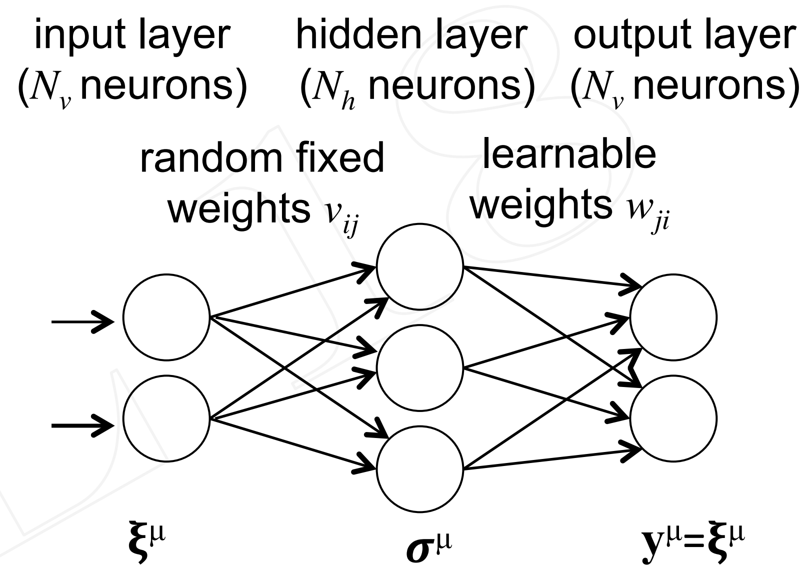
$$\langle\!\langle \log \Omega \rangle\!\rangle = \lim_{n\to 0} \frac{\langle\!\langle \Omega^n \rangle\!\rangle - 1}{n}, \quad \text{critical capacity: } \alpha_c = \lim_{N\to\infty} \frac{p_c}{N}$$

- Perceptron learning rule ($\kappa=0$): $\Delta w_i = \eta \xi_i \,(d^{\mu} - y^{\mu})$

A simplified expansive (over-complete) autoencoder

- Binary neurons (± 1)
- Expansion ratio: $\Lambda = N_h / N_v$
- Fixed encoding weights v_{ij} are randomly sampled from $\mathcal{N}(0, 1)$
- Goal: reconstruct random patterns $\{\boldsymbol{\xi}^\mu\}_{\mu=1,\dots,p}$ by learning the decoding weights w_{ji}
- Perceptron learning rule: $\Delta w_{ji} = \eta(\xi_j^\mu - y_j^\mu)\sigma_i^\mu$
- Dense coding level for patterns: $P(\xi_i = +1) = 0.5$
- Coding level of hidden layer: $P(\sigma_i = +1) = f$
- Maximal/critical storage Capacity:
  $\alpha_{max} = p_{max} / N_h$ as $N_h \longrightarrow \infty$
- Storage criteria: meeting fixed-point equations

$$\forall j, \mu: \quad \xi_j^\mu = \operatorname{sgn}\left(\sum_i w_{ji} \operatorname{sgn}\left(\sum_l v_{il}\xi_l^\mu\right)\right)$$



Dynamics:

$$\sigma_i^\mu = \operatorname{sgn}\left(\sum_{j=1}^{N_v} v_{ij}\xi_j^\mu - \theta\right)$$

$$y_j^\mu = \operatorname{sgn}\left(\sum_{i=1}^{N_h} w_{ji}\sigma_i^\mu\right)$$

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A mean-field approximation (MFA)

$$\xi_j^\mu = \mathrm{sgn}\left(\sum_{i=1}^{N_h} w_{ji}\mathrm{sgn}\left(\sum_{l=1}^{N_v} v_{il}\xi_l^\mu\right)\right)$$

Approximated by a *quenched* random variable with a Gaussian distribution : $\mathcal{N}(0, N_v)$

$$= \mathrm{sgn}\left(\sum_{i=1}^{N_h} w_{ji}\mathrm{sgn}\left(\boxed{\sum_{l\neq j;l=1}^{N_v} v_{il}\xi_l^\mu} + v_{ij}\xi_j^\mu\right)\right)$$

$$= \mathrm{sgn}\left(\sum_{i=1}^{N_h} w_{ji}\mathrm{sgn}\left(z_i^\mu + v_{ij}\xi_j^\mu\right)\right)$$

$$\mathrm{P}\left(\sigma_i^\mu \middle| \xi_j^\mu\right) \simeq \frac{1}{2} + \sigma_i^\mu \xi_j^\mu \frac{v_{ij}}{\sqrt{2\pi N_v}}$$

$$\left(\sigma_i^\mu \perp \sigma_k^\mu\right) \middle| \, \xi_j^\mu \quad \Rightarrow \quad \mathrm{P}(\boldsymbol{\sigma}^\mu | \xi_j^\mu) = \prod_i \mathrm{P}(\sigma_i^\mu | \xi_j^\mu)$$

A mean-field approximation (MFA)

Probability distribution

$$\mathrm{P}\left(\sigma_i^\mu \middle| \xi_j^\mu\right) \simeq \frac{1}{2} + \sigma_i^\mu \xi_j^\mu \frac{v_{ij}}{\sqrt{2\pi N_v}}$$

$$\left(\sigma_i^\mu \perp \sigma_k^\mu\right) \middle| \, \xi_j^\mu \quad \Longrightarrow \quad \mathrm{P}(\boldsymbol{\sigma}^\mu | \xi_j^\mu) = \prod_i \mathrm{P}(\sigma_i^\mu | \xi_j^\mu)$$

Mean-Field Approximation (MFA) for the *replica* calculation

Gardner volume:

$$\Omega = \int_{\|\mathbf{w}\|^2=N_h} d^{N_h}\mathbf{w} \prod_{\mu=1}^{p} \Theta\Big(\xi_j^\mu \frac{1}{\sqrt{N_h}} \sum_{i=1}^{N_h} w_{ji}\sigma_i^\mu - \kappa\Big)$$

Replica theory: compute $\langle\!\langle \log(\Omega) \rangle\!\rangle$ over distribution of patterns using the replica method

$$\langle\!\langle \log \Omega \rangle\!\rangle = \lim_{n\to 0} \frac{\langle\!\langle \Omega^n \rangle\!\rangle - 1}{n}$$

Probability distribution

$$\mathrm{P}\big(\sigma_i^\mu \big| \xi_j^\mu\big) \simeq \frac{1}{2} + \sigma_i^\mu \xi_j^\mu \frac{v_{ij}}{\sqrt{2\pi N_v}}$$

$$\big(\sigma_i^\mu \perp \sigma_k^\mu\big) \,\big|\, \xi_j^\mu \quad \Longrightarrow \quad \mathrm{P}(\boldsymbol{\sigma}^\mu | \xi_j^\mu) = \prod_i \mathrm{P}(\sigma_i^\mu | \xi_j^\mu)$$

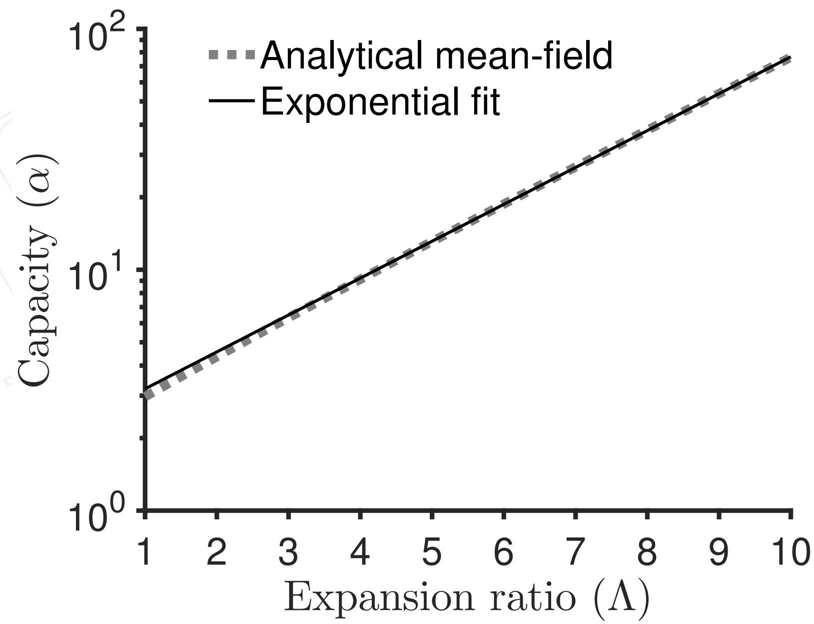
Exponential critical capacity in the MFA

Solutions (replica-symmetric, locally stable):

$$\boxed{\begin{aligned}\alpha_c^{\mathrm{MFA}} \int_{M\sqrt{2\Lambda/\pi}-\kappa}^{\infty} Dt\left(\kappa + t - \sqrt{2\Lambda/\pi}\right)^2 &= 1 - M^2 \\ \alpha_c^{\mathrm{MFA}} \int_{M\sqrt{2\Lambda/\pi}-\kappa}^{\infty} Dt\left(\kappa + t - \sqrt{2\Lambda/\pi}\right)\sqrt{2\Lambda/\pi} &= M,\end{aligned}}$$

where $M = \sum_i \frac{v_i w_i}{N_h},\ \Lambda = \frac{N_h}{N_v}$

$$Dt \equiv \frac{dt}{\sqrt{2\pi}} \mathrm{e}^{\frac{-t^2}{2}}$$



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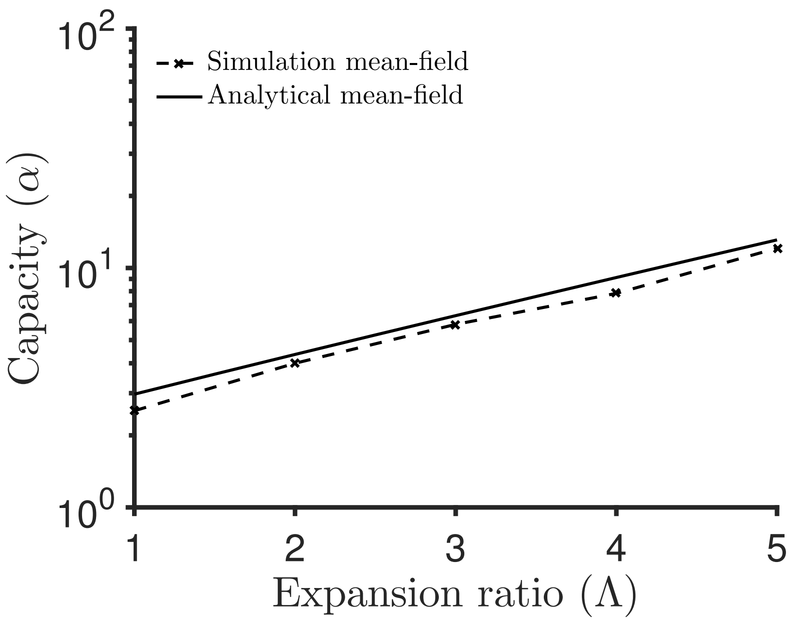
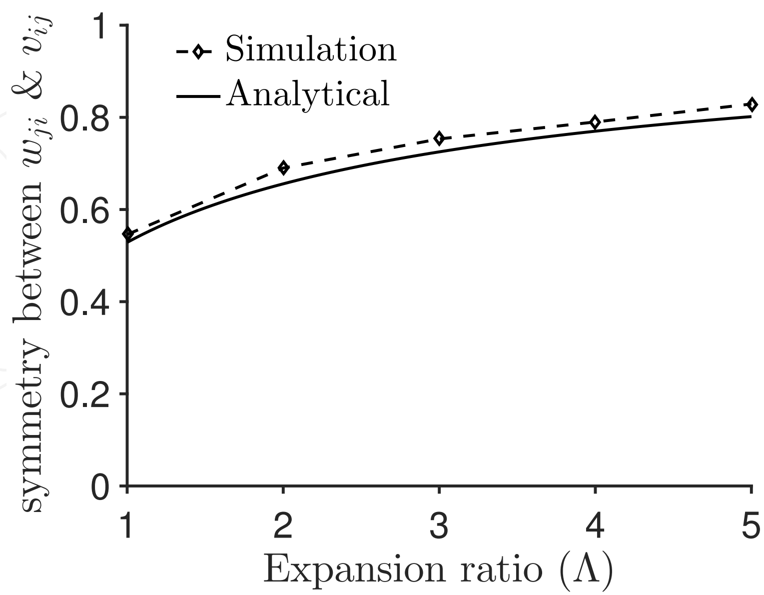
Comparison with simulation (perceptron learning rule)





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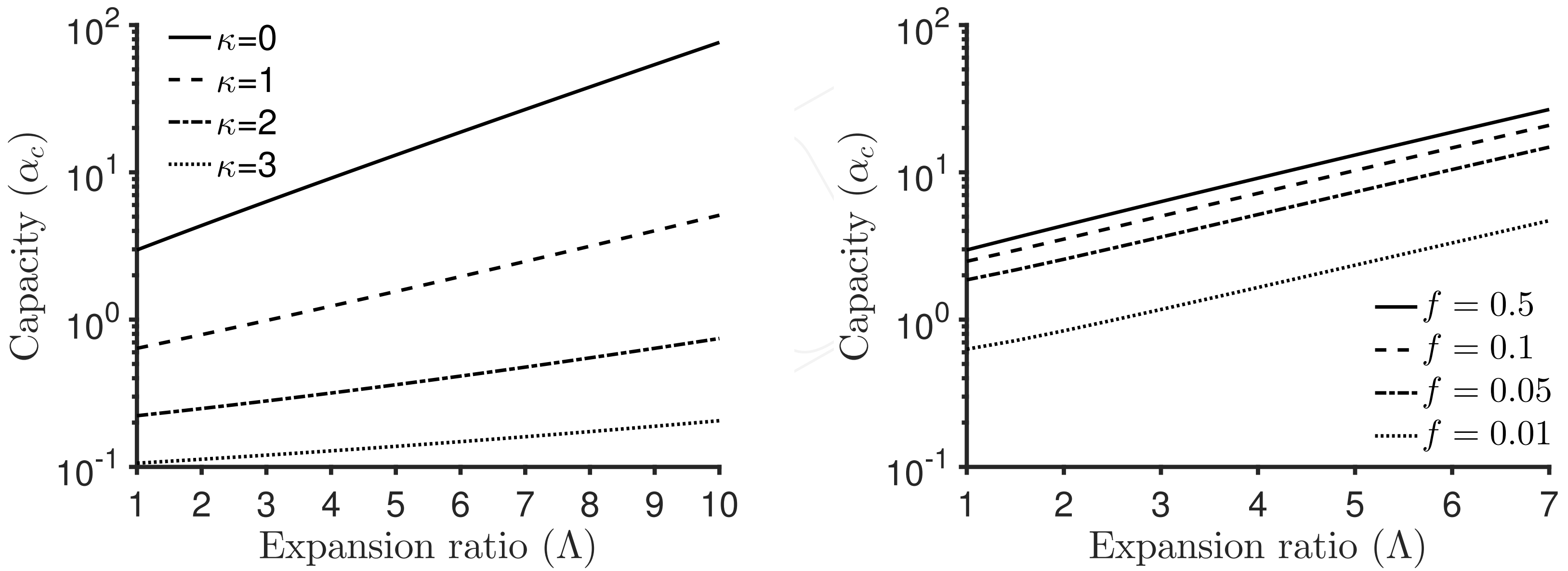
Effect of robustness of output, sparseness in the hidden layer



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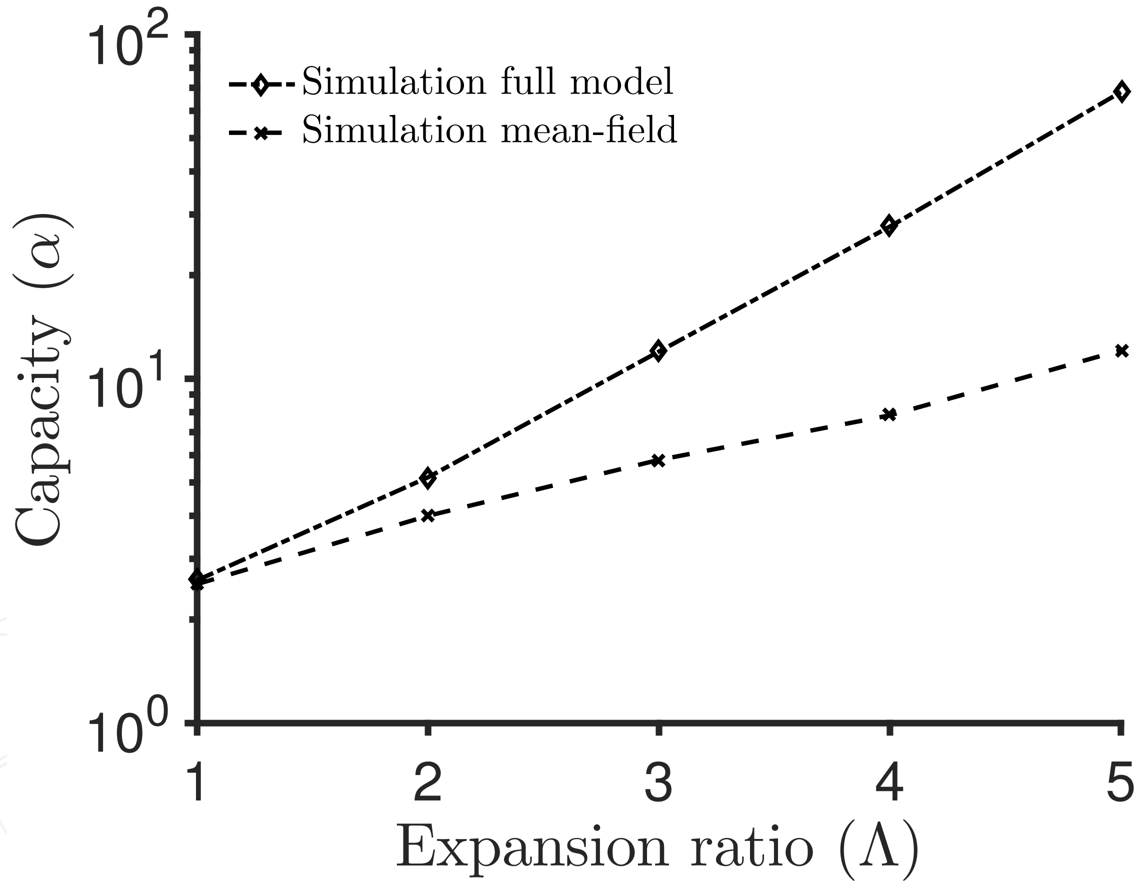
Comparison with the full-model



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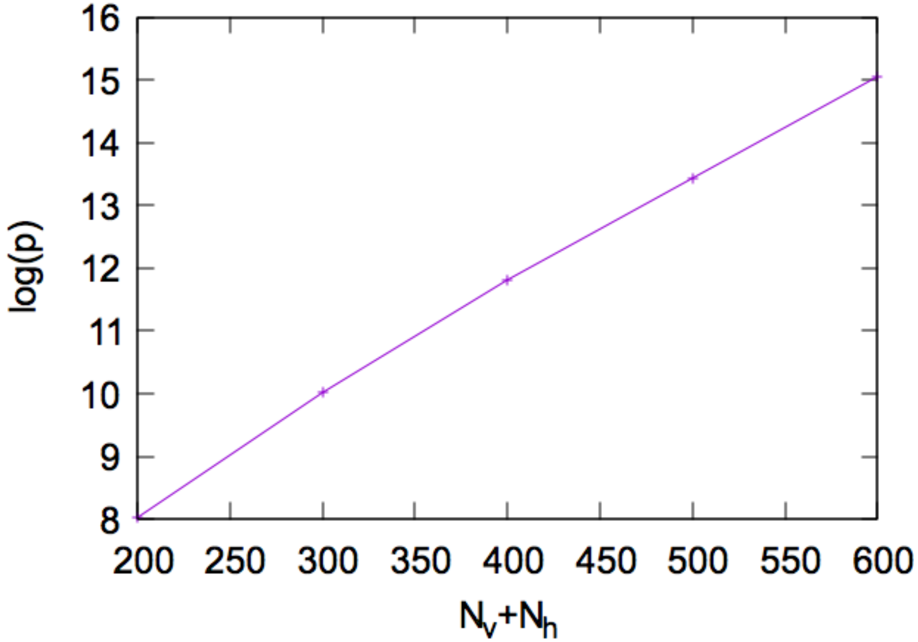
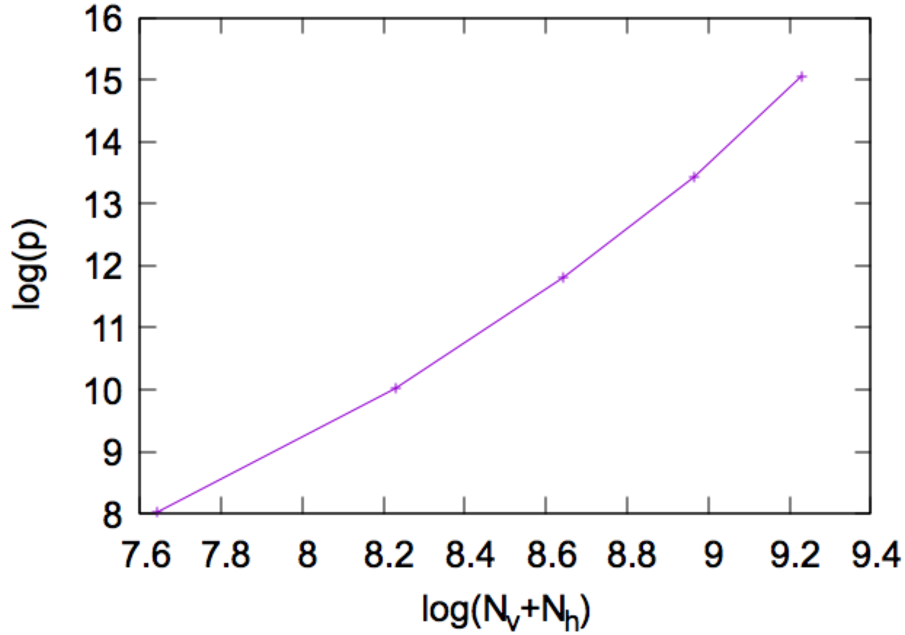
Log of number of patterns vs. total number of neurons





Discussion

- Expansive representation has important computational implications.
- *Exponential* scaling of the capacity with the expansion ratio in our autoencoder
  - Expansion makes up for the loss of information due to binarization
- In very good agreement with results of simulations using an online learning rule
- Future directions
  - Robustness to noise by training encoding weights
  - Computing the capacity of the full autoencoder model
  - Extension to the capacity of MLP and deep nets

Acknowledgement

Alia Abbara

Discussion with many colleagues …

Question?